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NUMERICAL COMPUTATION OF CAPILLARY
SURFACES ON IRREGULARLY SHAPED DOMAINS BY A
FINITE ELEMENT METHOD

Norman Albright

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Norman Albright

Lawrence Berkeley Laboratory
University of California
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ABSTRACT

In this report we explore the nature of capillary surfaces on several noncircularly symmetric domains and investigate the suitability of the computer program JASON for calculating these surfaces. We investigate how the accuracy of the computed solution depends on various parameters. We calculate capillary surfaces for elliptical cross sections. We describe a procedure for calculating surfaces on cross sections with corners for values of the contact angle less than the critical value. We use this method to calculate surfaces on a square cross section and on a circular cross section with a reentrant notch.

1. INTRODUCTION

In this report we explore the nature of capillary surfaces on various noncircularly symmetry domains and investigate the suitability of the computer program JASON for calculating these surfaces.

In the next section we define the capillary surface problem for liquids with contact angle γ between 0° and 90° . The surface satisfies a pair of equations, Eqs. (1) and (2). In the following section we point out some elementary properties of these equations. Next we state some theorems first proved in Ref. 1 for the nonexistence of solutions to Eqs. (1) and (2) in a zero gravitational field. If the curvature of the perimeter of the domain is sufficiently large at a point, then there exists a critical contact angle such that Eqs. (1) and (2) have no solution for $\gamma < \gamma_{\text{crit}}$. We give the value of γ_{crit} for a sharp corner and a lower bound on γ_{crit} for a rounded corner. We then describe the nature of the solutions in a nonzero gravitational field.

Next we describe JASON, a general purpose computer program that solves second-order elliptic partial differential equations in two dimensions on a nonuniform quadrilateral mesh by a finite element method. JASON is reliable and easy to use, but it is not necessarily the most efficient program for this problem, since it is designed for a very general class of problems.

We consider the system of discrete equations corresponding to Eqs. (1) and (2) for a particular mesh. We study how the number of iterations and computer time required to solve the discrete equations depend on the mesh spacing for uniform meshes. Next we explore how the accuracy of the computed solution varies over the cross section with the mesh spacing

and with the contact angle, on a square cross section for the case of zero gravity. A closed-form solution to Eqs. (1) and (2) is known for this case.

Next we calculate capillary surfaces on elliptical cross sections. We investigate how the height at various points on the cross section depends on the contact angle and the ratio of the major and minor axes. Numerical estimates of γ_{crit} are obtained and compared with the lower bounds mathematically derived from a theorem given in Ref. 1.

We describe a procedure for calculating capillary surfaces on cross sections with sharp corners for values of γ less than γ_{crit} . We use this method to calculate surfaces on a square cross section and on a circular cross section with a reentrant notch. Finally, we discuss how the height of the surface at various points on these cross sections depends on the contact angle.

2. DEFINITION OF THE PROBLEM

We consider the equilibrium free surface of a liquid partly filling a vertical cylinder for the case in which the surface height $u(x,y)$ is a single-valued smooth function of x and y and in which there is sufficient liquid to cover the base of the cylinder entirely. The gravitational field is taken to be positive when directed vertically downward. The height then satisfies the equation

$$\nabla \cdot \left(\frac{1}{W} \nabla u \right) = \kappa u + 2H \quad (1)$$

$$W = (1 + |\nabla u|^2)^{\frac{1}{2}},$$

where ∇ is the two-dimensional operator $(\partial/\partial x, \partial/\partial y)$, $\kappa = \rho g/\sigma$ is the capillary constant, ρ is the difference in densities between the liquid and gas phases, g is the acceleration due to gravity, and σ is the gas-liquid surface tension. The constant $2H$ is determined by the cross-sectional shape of the cylinder, the volume of the liquid, and the boundary condition satisfied by the free surface of the liquid at the cylinder wall.

The boundary conditions for a free surface that makes a contact angle γ with the cylinder wall is

$$\frac{1}{W} \frac{\partial u}{\partial n} = \cos \gamma \quad \text{at the wall,} \quad (2)$$

where $\partial u/\partial n$ denotes the derivative of u with respect to the outward directed normal at the wall. Only the case of wetting liquids, $0^\circ \leq \gamma < 90^\circ$, will be considered here. (The nonwetting case can be obtained from it directly by means of a simple transformation.)

3. ELEMENTARY PROPERTIES

The quantity $\nabla \cdot (W^{-1} \nabla u)$ in Eq. (1) is twice the mean curvature of the surface $z = u(x, y)$. Thus in a zero-gravity field ($\kappa = 0$) the free surface has constant mean curvature.

If one integrates Eq. (1) over the cross section of the cylinder, and uses Eq. (2), one obtains

$$\kappa A \bar{u} + 2HA = L \cos \gamma, \quad (3)$$

where $\bar{u} = A^{-1} \int_{\Omega} u \, dx \, dy$ is the average height of the free surface, and A and L are the area and perimeter, respectively, of the cross section Ω .

For the case $\kappa \neq 0$, if $u(x,y)$ is a solution of Eqs. (1) and (2) for one value of H , then $u(x,y)$ plus a constant is a solution for any other value of H . The solution is unique for a particular value of H if $\kappa \geq 0$. The value of H is related to the reference level from which the height of the capillary surface is measured. It is sometimes convenient to measure the height of the surface from the level of an infinite reservoir into which the cylinder, without bottom, is dipped. On the surface of the reservoir, infinitely far from the cylinder, $u=0$, $\nabla u=0$, and therefore $H=0$. The average height $\bar{u}_0$ to which the capillary surface inside the cylinder rises above the reservoir is then obtained from Eq. (3).

$$\bar{u}_0 = (L \cos \gamma) / \kappa A .$$

For the case $\kappa=0$, one cannot arbitrarily choose H . It is determined by Eq. (3).

$$2H = (L \cos \gamma) / A . \quad (3)$$

For $\kappa=0$, the solution of Eqs. (1) and (2) is determined only up to an additive constant. A convenient way to choose this constant is to take $u=0$ at the lowest point of the capillary surface. For uniformity all the numerical results presented in this report will use this choice for $u=0$, both for the case $\kappa=0$ and for $\kappa \neq 0$. This will enable us to compare directly calculations for different values of κ .

4. NONEXISTENCE OF SOLUTIONS FOR THE CASE $\kappa = 0$

For each cylinder, there may exist a critical contact angle such that Eqs. (1) and (2) have no solution for $0 \leq \gamma < \gamma_{\text{crit}}$. Several important theorems have been formulated in Refs. 1,4 that relate γ_{crit} to the shape of the cross section of the cylinder. We give below forms of them relevant to our problem.

Theorem 1. Let the cross-section boundary have a corner with an interior angle 2α . Then a solution of Eqs. (1) and (2) can exist in the neighborhood of that corner only if

$$\gamma \geq 90^\circ - \alpha$$

and no solution exists if

$$\gamma < 90^\circ - \alpha.$$

Example: $\alpha = 45^\circ$ for a square cross section; thus the critical contact angle is $\gamma_{\text{crit}} = 45^\circ$. There is no solution for $0 \leq \gamma < \gamma_{\text{crit}}$.

A similar result holds for a region on a curved boundary on which the curvature is large relative to a value determined by the entire cross section.

Theorem 2. Suppose there is a point p on the boundary at which the curvature is greater than L/A ; then there exists a critical contact angle such that there is no solution of Eqs. (1) and (2) in a neighborhood of p for $0 \leq \gamma < \gamma_{\text{crit}}$.

Example: Let the cross section be an ellipse. The curvature of an ellipse is greatest at the point where the semimajor axis cuts the boundary. The curvature at this point exceeds L/A when the ratio b of semiminor

and semimajor axes is less than 0.6116. According to Theorem 2, there exists a critical contact angle for an ellipse with $b < 0.6116$ [2].

A third theorem gives a lower bound for γ_{crit} . Consider the cross section of a cylinder shown in Fig. 1. Let A be the area of the entire cross section, and L be its perimeter. Let the cross section be cut by a curve Γ , which intersects the perimeter at points p_1 and p_2 . The curve Γ divides the area of the cross section into two parts, A^* and $A - A^*$, and divides the perimeter into two parts, L^* and $L - L^*$. Let $|\Gamma|$ denote the length of the curve Γ from p_1 to p_2 . Then the following theorem holds [1].

Theorem 3. Let V be the function

$$V = \frac{|\Gamma|A}{|L^*A - A^*L|} \quad ; \quad (4)$$

then

$$\cos \gamma_{\text{crit}} \leq V_0 \quad ,$$

where V_0 is the minimum of V with respect to all possible curves Γ .

This minimization can be done in two steps. First, find the Γ that minimizes V for a fixed pair of intersection points, p_1 and p_2 ; then vary p_1 and p_2 .

For any p_1 and p_2 , the Γ that minimizes V is an arc of a circle with radius

$$R = \frac{A}{LV_p(p_1, p_2)} \quad , \quad (5)$$

where $V_p(p_1, p_2)$ is the minimum of V for fixed p_1 and p_2 [2].

solution of Eqs. (4) and (5) gives $V_p(p_1, p_2)$. Finally, minimization of $V_p(p_1, p_2)$ with respect to p_1 and p_2 gives V_0 .

Example: The lower bounds for γ_{crit} for ellipses with ratio b of semiminor and semimajor axes are:

b	Bound
0.20	35.12°
0.25	26.95°
0.33	16.88°
0.40	10.32°
0.50	3.71°
0.60	0.12°

Numerical solution of Eqs. (1) and (2) indicates that these bounds are close to γ_{crit} .

5. BEHAVIOR OF SOLUTIONS FOR THE CASE $\kappa \neq 0$

For the case $\kappa \neq 0$, Eqs. (1) and (2) have a solution for each γ . However, the behavior of the solution is different for $\gamma < \gamma_{\text{crit}}$ and $\gamma \geq \gamma_{\text{crit}}$ [3].

Theorem 4. Let the cross-section boundary have a corner with an interior angle 2α . Let ρ and θ be polar coordinates centered at the corner with θ measured from the bisector of the corner angle. Let

$$q = \frac{\cos \gamma}{\sin \alpha} = \frac{\cos \gamma}{\cos \gamma_{\text{crit}}},$$

where $\gamma_{\text{crit}} = 90^\circ - \alpha$, as in the case $\kappa = 0$. If $\gamma \geq \gamma_{\text{crit}}$, then $u(\rho, \theta)$ is bounded in the neighborhood of the corner.

If $0 \leq \gamma < \gamma_{\text{crit}}$, then $u(\rho, \theta)$ is asymptotic to

$$u(\rho, \theta) \sim u_0(\rho, \theta) + [q \cos \theta - (1 - q^2 \sin^2 \theta)^{\frac{1}{2}}] / \kappa \rho \quad (6)$$

as $\rho \rightarrow 0$, where u_0 is $O(1)$. Inside the cylinder u grows like $1/\rho$ as the corner is approached.

The solution in a cylinder with a curved boundary is bounded for all γ . However, this bound depends inversely on the radius of the corner [4].

Theorem 5. Let C be the maximum curvature of the cross-section boundary, and let $r = 1/C$. Then in a neighborhood of the corner

$$u(x, y) < r + \frac{2}{\kappa r} \quad (7)$$

6. JASON

The computer program JASON solves the nonlinear elliptic partial differential equation in two independent variables [5]:

$$\nabla \cdot (c \nabla \phi) = a \phi + b \quad (8)$$

with boundary condition:

$$c \nabla \phi \cdot \hat{n} = f \phi + g, \quad (9)$$

where $a = a(x, y)$, $b = b(x, y)$, $c = c(x, y, |\nabla \phi|^2)$, $f = f(s)$, $g = g(s)$, and s is the arc length along the boundary. It uses a bilinear finite element method on a nonuniform quadrilateral mesh. The resulting algebraic system of equations is solved by the one-step block successive over-relaxation-Newton method (BSOR-Newton).

The domain of a problem suitable for JASON can be composed of one or more distinct subregions separated by common boundaries. Each subregion

can have different functions a , b , and c . If the values of a , b , and c for a particular subregion are constant, they can be specified on a data card; if they are functions of x , y , or $|\nabla\phi|^2$, JASON must be supplied with a subroutine to calculate them. One can suppress solution of Eq. (8) in a particular subregion by specifying $c=0$ in that subregion.

JASON contains a mesh generator that produces a smooth mesh by "equipotential zoning." Input to the mesh generator consists of the set of boundary points of each subregion. Each point is specified by four numbers: the x and y coordinates of the point, and the (integer) L and M values of mesh line coordinates through the point. One need not specify every boundary point. JASON will compute by linear interpolation the boundary points that have been skipped, if they lie on the same mesh line.

Dirichlet boundary conditions can be imposed at any point in the mesh. Neumann boundary conditions are restricted to the boundary of the entire domain of the problem and the boundaries between subregions with $c=0$ and those with $c \neq 0$.

Before using JASON, one should make a rough sketch of the desired mesh, to guide the choice of the boundary points. These define a polygon whose boundary approximates that of the original domain. For the case $\kappa=0$, one must calculate the perimeter and area of this polygon, in order to calculate H .

The input to JASON is a series of data cards. The first card specifies the procedures to be performed: generate a mesh, plot the mesh, solve Eq. (8) for ϕ , calculate $\nabla\phi$, and plot ϕ . The second card is the title for printed and plotted output. The third card gives

-11-

the size of the mesh for the entire domain, LMAX and MMAX. The mesh coordinates take the values $1 \leq L \leq \text{LMAX}$ and $1 \leq M \leq \text{MMAX}$.

The next input is a set of cards for each subregion. The first card of each set lists the values of a , b , and c for a subregion, or provides parameters for a subroutine that calculates a , b , and c . The remaining cards of the set give the boundary points of that subregion.

The next cards contain the values of L , M , f , and g at enough points to specify the boundary conditions. If f and g are constant along a boundary, one needs to give only L , M , f , and g at the first boundary point and L and M at the subsequent corners of that boundary.

The next card allows one to choose the iteration control parameters of the solution subroutines. The remaining cards specify the domains for which the values of ϕ or $\nabla\phi$ are to be printed or the domain in which ϕ is to be plotted.

7. SQUARE CROSS SECTION WITH $\kappa=0$ AND $\gamma \geq \gamma_{\text{crit}}$

The convergence properties of JASON were studied by calculating the capillary surfaces for $\kappa=0$ in a cylinder with a square cross section. The exact solution is known for $45^\circ \leq \gamma \leq 90^\circ$ and is a portion of a lower hemisphere. The square had an edge of length 2 and was centered at the origin. It was the domain $-1 \leq x \leq 1$ and $-1 \leq y \leq 1$. Figure 2 shows the height of the capillary surface along the edge of the square $x=1$ for contact angles $\gamma=45^\circ$, 50° , 55° , and 60° . For $\gamma=\gamma_{\text{crit}}=45^\circ$, the slope is infinite at the corner $x=1$ and $y=1$, although the rise height is finite.

The same data are graphed in a different way in Fig. 3. This figure shows how the height at several fixed points on the edge of the square varies with the contact angle γ . For $\gamma = 90^\circ$ the surface is flat. Figure 3 shows that the height in the corner increases rapidly as γ nears γ_{crit} . The height at other points on the edge varies much less rapidly with γ .

The coordinate axes $x=0$ and $y=0$ are lines of reflection symmetry, so the solution in one quadrant repeats in the other three quadrants. The solution was calculated in the first quadrant, $0 \leq x \leq 1$ and $0 \leq y \leq 1$. The boundary conditions are: $\hat{n} \cdot \nabla u = 0$ on the lines $y=0$ and $x=0$, and $(\hat{n} \cdot \nabla u)/W = \cos \gamma$ on the lines $x=1$ and $y=1$. Here $\hat{n}$ denotes the outward directed unit normal for each edge.

Capillary surfaces were calculated on uniform meshes with mesh spacing $h = 0.2, 0.1$, and 0.05 . Surfaces were calculated for contact angle $\gamma = 45^\circ, 50^\circ, 55^\circ$, and 60° for each mesh spacing.

Surfaces were also calculated using two nonuniform meshes, which were successive refinements of the uniform mesh with $h=0.05$. The refinements were made near the corner of the square. The first mesh (NU1) had $h=0.05$ for $0 \leq x \leq 0.8$ or $0 \leq y \leq 0.8$ and $h=0.025$ for $0.8 \leq x \leq 1.0$ or $0.8 \leq y \leq 1.0$. The second mesh (NU2) was a refinement of NU1 which had $h=0.0125$ for $0.9 \leq x \leq 1.0$ or $0.9 \leq y \leq 1.0$.

We now consider the number of relaxation cycles required to solve the system of discrete equations for a particular mesh. In subsequent paragraphs we will discuss how the solution of the discrete equations approaches the solution of Eqs. (1) and (2) as the mesh is refined.

The number of cycles required to solve the system of discrete equations depends on the mesh spacing. This was studied by calculating the surfaces for $\gamma = 50^\circ$ on a sequence of uniform meshes. Each mesh had n equally spaced horizontal mesh lines and n vertical mesh lines. The meshes were 6×6 , 11×11 , 16×16 , and 21×21 . JASON solves the discrete equations by the one-step block successive over-relaxation-Newton method, BSOR-Newton [6].

These results are compared with those of another program, which solves the discrete equations by a dynamic alternating direction implicit method, DADI [7]. Both computations were performed on a CDC 7600. The number of cycles and CPU-seconds required are shown in Table 1.

TABLE 1. Comparison of BSOR-Newton with DADI
on a square domain with n vertical and
 n horizontal mesh lines.

Method	Final R/L		$n = 6$	$n = 11$	$n = 16$	$n = 21$
BSOR-Newton	1×10^{-6}	Cycles used:	22	36	63	84
BSOR-Newton	1×10^{-6}	CPU-sec used:	0.615	3.660	13.152	30.018
DADI	1×10^{-8}	Cycles used:	12	16	18	24
DADI	1×10^{-8}	CPU-sec used:	0.023	0.088	0.204	0.465

The DADI method is approximately 18 times faster per cycle than JASON. However, JASON is a general-purpose program that solves the discrete equations on a nonuniform quadrilateral mesh, and would be expected to be slower than the DADI program, which was written specifically for a uniform rectangular mesh for this problem. JASON is reliable and easy to use, but is not necessarily efficient for this problem.

The number of cycles required for JASON to solve the discrete equations depends on the criterion for terminating the iteration and the procedure followed in optimizing the relaxation parameter ω . The termination criterion used here is that $R/L < 1 \times 10^{-6}$. R is the square root of the sum of the squares of the residual at each point. L is the square root of the sum of the squares at u at each point.

The initial value of ω is 1.5. This was used until R/L was less than 1×10^{-2} , then ω was adjusted upward toward the estimated asymptotically optimal value, half the estimated increment every five SOR iterations.

The number of cycles required depends on these iterations parameters. However, Table 1 gives a rough measure of the amount of computing necessary to solve the discrete equations, and how this depends on the mesh spacing.

The number of cycles required to solve the discrete equations depends only weakly on the contact angle γ . This can be seen by comparing the values of R/L for different γ after the same number of relaxation cycles. On a 21×21 uniform mesh, 80 cycles reduced R/L to 2.9×10^{-6} for $\gamma = 45^\circ$ and 2.1×10^{-6} for $\gamma = 60^\circ$. On an 11×11 uniform mesh, 30 cycles reduced R/L to 15.0×10^{-6} for $\gamma = 45^\circ$ and 8.7×10^{-6} for $\gamma = 60^\circ$. This weak dependence on γ is shown in more detail in Table 2.

Table 2. $R/L \times 10^{-6}$ after n cycles for various γ .

Mesh	Cycles	$\gamma = 45^\circ$	$\gamma = 50^\circ$	$\gamma = 55^\circ$	$\gamma = 60^\circ$
11x11	30	15.0	12.5	10.3	8.7
21x21	80	2.9	2.6	2.3	2.1

Table 3 shows an experimental study of the convergence of the solution of the discrete equations toward the known solution of Eqs. (1) and (2) as the mesh spacing decreases. The tabulated quantity δu is the difference between the known solution and the solution computed with a particular mesh. It is tabulated as a function of contact angle γ , mesh spacing h , and position y along the edge of the square. The point $y=1$ is the corner, and $y=0$ is the midpoint of the full square.

Table 3 shows that for fixed values of γ and h , δu is larger for y near the corner. It further shows that for fixed values of y and h , δu is larger for γ near 45° .

In the remaining paragraphs, we shall discuss how δu changes with h for fixed values of γ and y . We consider first the uniform meshes. Table 3 shows that for $0 \leq y \leq 0.9$, δu decreased by $1/4$ when h was decreased by $1/2$. That is, δu is proportional to h^2 for these values of y on uniform meshes. However, δu decreased less rapidly than h^2 at the corner $y=1$. Convergence is poorer at the corner probably because the slope is very large there.

We consider next the nonuniform meshes. The mesh NU1 has $h=0.05$ for $0 \leq y \leq 0.8$ and $h=0.025$ for $0.8 \leq y \leq 1.0$. We shall compare the δu on NU1 with that on the uniform mesh with $h=0.05$. For both the 45° and 50° cases, δu decreased for $0.9 \leq y \leq 1.0$, δu was about the same for $y=0.85$, δu increased for $y=0.8$, and δu was about the same for $0 \leq y \leq 0.6$. That is, δu decreased in the upper half of the refined region, increased at the boundary of the refined and unrefined regions, and was about the same in the interior of the unrefined region.

The mesh NU2 has $h=0.0125$ for $0.9 \leq y \leq 1.0$ and has h the

TABLE 3. $\delta u \times 10^5$ for $x=1.0$ and $0 \leq y \leq 1.0$.

h	y = 1.0	0.95	0.9	0.85	0.8	0.6	0.4	0.2	0.0
$\gamma = 45^\circ$									
0.2	34166				2051	487	198	108	84
0.1	26689		2114		473	102	46	26	20
0.05	20944	2239	515	161	77	25	12	7	5
NU1	16761	832	220	172	140	33	11	6	2
NU2	13478	434	291	217	194	29	6	3	2
$\gamma = 50^\circ$									
0.2	4186				831	295	143	86	70
0.1	1804		503		209	73	35	21	17
0.05	701	258	125	75	51	19	9	5	5
NU1	304	117	81	71	64	20	8	5	4
$\gamma = 55^\circ$									
0.2	1468				391	173	94	60	50
0.1	529		188		101	44	23	14	12
0.05	176	78	48	33	26	11	6	4	3
$\gamma = 60^\circ$									
0.2	605				192	97	57	39	33
0.1	199		82		50	25	14	10	8
0.05	62	31	21	16	13	6	4	3	2

same as NU1 for other values of y . We shall compare the δu on NU2 with that on NU1. It decreased for $0.95 \leq y \leq 1.0$, increased for $0.8 \leq y \leq 0.9$, and was about the same for $0 \leq y \leq 0.6$. That is, δu decreased in the upper half of the refined region, increased in the region of intermediate mesh spacing, and was about the same in the region with $h = 0.05$.

8. ELLIPTICAL CROSS SECTION

Capillary surfaces were calculated for cylinders of elliptical cross section with semimajor axis $a = 1.0$ and semiminor axes $b = 0.60, 0.33$, and 0.20 . The cases $b = 0.60$ and 0.33 were calculated for $\kappa = 0$. The case $b = 0.20$ was calculated for both $\kappa = 0$ and $\kappa = 1$. Closed form solutions are not known for the ellipse as they are for the square for $\kappa = 0$.

Figure 4 shows how a quadrilateral mesh was fit to $1/4$ of an ellipse. The $1/4$ ellipse was made into a four "sided" figure by choosing a point on the curved edge and using it as a fourth corner. A mesh was fit to this by taking one pair of opposite sides to be mesh lines with constant mesh coordinate L , and the other pair to be mesh lines with constant coordinate M .

Figures 5 and 6 show the 11×6 meshes generated for the cases $b = 0.33$ and 0.20 . Figure 7 shows the 21×11 mesh generated for $b = 0.20$. Figure 8 shows the level curves of the capillary surface for the case $b = 0.33$ and $\gamma = 60^\circ$.

According to Theorem 2 there will be a critical contact angle if

the curvature at any point on the ellipse exceeds the ratio of its perimeter to its area. This occurs if $b/a < 0.6116$. Theorem 3 gives a lower bound for the critical angle. These are shown in Table 4. For the case $\kappa=0$, capillary surfaces exist for $\gamma \geq \gamma_{\text{crit}}$, but not for $\gamma < \gamma_{\text{crit}}$. For $\kappa \neq 0$, capillary surfaces exist and are bounded for $\gamma < \gamma_{\text{crit}}$, but the bound is inversely related to both κ and the maximum radius of curvature of the ellipse, as in Eq. (7).

Theorems 2 and 3 restrict the existence of capillary surfaces for a cross section with a smoothly curved boundary. However, the actual cross section that is used is not an ellipse, but a polygonal approximation to an ellipse. Because of this, Theorem 1 gives an additional existence criterion, which depends on the interior angles at the polygon's corners. By Theorem 1 the critical angle is $\gamma_{\text{crit}} = 90^\circ - \alpha$, where 2α is the smallest interior angle. The γ_{crit} from Theorem 1 are shown in Table 4.

Theorems 1, 2, and 3 limit the existence of solutions of the differential Eqs. (1) and (2). However, the discrete system of equations approximating (1) and (2) can have a solution even when Eqs. (1) and (2) do not. This is worth remembering because the 11×6 meshes used to explore the ellipse problem are rather coarse, especially for the largest ellipse, $b=0.60$. Thus the local truncation error, which is of the order of the mesh spacing squared, is not very small.

The computing times used to calculate the various capillary surfaces are shown in Table 5. For the $\kappa=0$ cases, the smallest time was for the largest contact angle. For example, for the $b=0.60$ case, with the 11×6 mesh, 1.13 CPU seconds were used to calculate the surface for $\gamma=40^\circ$, and 1.57 CPU seconds were used for $\gamma=0^\circ$. However, for the $\kappa=1$ case, the smallest time was for the smallest γ . Note that it took approximately

TABLE 4. γ_{crit} from Theorems 1 and 2 for various meshes and values of b .

b	Mesh	γ_{crit}	
		Theorem 3	Theorem 1
0.60	11×6	$\geq 0.12^\circ$	8.79°
0.60	21×11	$\geq 0.12^\circ$	4.55°
0.33	11×6	$\geq 16.88^\circ$	15.71°
0.20	11×6	$\geq 35.12^\circ$	24.89°
0.20	21×11	$\geq 35.12^\circ$	13.43°

TABLE 5. CPU-sec used for various meshes and values of b .

b	κ	Mesh	CPU - sec
0.60	0	11×6	1.13 - 1.57
0.60	0	21×11	19.23 - 19.39
0.33	0	11×6	3.66 - 6.24
0.20	0	11×6	6.20 - 11.60
0.20	0	21×11	44.70 - 71.57
0.20	1	11×6	7.71 - 9.38

the same time to compute surfaces for the ellipse with its irregular mesh as for the rectangle with its regular mesh. The rectangle with 64 mesh points took 1.22 CPU seconds. The ellipse with the 11×6 mesh took 1.13-1.57 CPU seconds for the $b = 0.60$ case. The $b = 0.33$ and 0.20 cases took more time, but these surfaces had steep gradients.

The computing time depends on the iteration control parameters. Because the 11×6 mesh is rather coarse, $R/L < 1.0 \times 10^{-4}$ was used in most calculations for the criterion for terminating the iteration. For the 21×11 mesh a stronger criterion was used, $R/L < 1.0 \times 10^{-5}$. The default value that JASON assumes is 1.0×10^{-6} .

Three iteration parameters can be chosen to attempt the minimization of the computing time. They are: the initial value of ω , the value of R/L at which one begins to adjust ω towards its estimated optimal value, and the fraction of the distance moved toward this value. The default values of these parameters are 1.5, 1.0×10^{-3} , and 0.06. However, it was found that for most of the capillary surface calculations, JASON can solve the discrete system of equations if the values 1.5, 1.0×10^{-2} , and 0.60 are used. Computing time is less with these values because fewer steps are used before changing ω and optimization is pursued more vigorously.

JASON prints the values of R/L and other quantities at every tenth iteration. If the solution attempt fails, one can examine this sequence of values and decide how to change the iteration control parameters. If R/L increases during the cycles when the initial ω is being used, then the initial ω should be reduced, say to 1.2. If R/L decreases while the initial ω is being used, but increases after optimization begins,

the fraction for the ω optimizer should be reduced. If this does not succeed, it may be necessary to reduce the value of R/L at which optimization begins.

Figure 9 shows the height of the capillary surfaces at the point A where the semimajor axis intersects the cylinder wall. Figure 10 shows the height at the point B where the semiminor axis intersects the cylinder wall. The height is taken to be zero at the center of the elliptical cross section. Figures 9 and 10 show $u(A)$ and $u(B)$ as a function of the contact angle γ for the four cases: $b=0.20$, 0.33 and 0.60 each with $\kappa=0$, and $b=0.20$ with $\kappa=1$. Figure 9 shows that for fixed γ , $u(A)$ is larger for smaller values of the semiminor axis b , while Fig. 10 shows that for fixed γ , $u(B)$ is larger for larger values of b .

We shall discuss first the case $b=0.20$ with $\kappa=0$. In this case the effect of the curvature of the actual ellipse near its major axis can be distinguished from the effect of the corner at point A of the polygonal approximation to the ellipse. The corner by itself would cause a γ_{crit} of 24.89° for the 11×6 mesh and one of 13.43° for the 21×11 mesh. However, the ellipse's curvature overwhelms this effect and causes a $\gamma_{\text{crit}} \geq 35.12^\circ$. Figure 9 shows that $u(A)$ becomes large with increasing rapidity as γ approaches 35° . Furthermore, when the mesh is refined from 11×6 to 21×11 , the value of $u(A)$ at 35° increases by 12%, while that at 40° increases by less than 1%. This must be the effect of the ellipse's curvature, since the effect of the approximating polygon's corner is reduced for the refined mesh. This indicates that the γ_{crit} due to the ellipse's curvature is near 35° , and that the lower bound given by

Theorem 3 is indeed close to γ_{crit} .

Consider next the case $b=0.20$ with $\kappa=1$. The capillary surface for a smooth ellipse is bounded at A because it has finite curvature. However, $u(A)$ should become infinite for γ less than the γ_{crit} of the approximating polygon's corner. Figure 9 shows that $u(A)$ for the 11×6 mesh becomes larger as γ approaches 25° , as is expected. Although the values of $u(A)$ are quite different for the cases $\kappa=0$ and $\kappa=1$, the values of $u(B)$ are almost the same. At 35° they differ by only 0.3%.

For the case $b=0.33$ with $\kappa=0$, the effects of the ellipse's curvature and the approximating polygon's corner cannot be distinguished for the 11×6 mesh. The first predicts a $\gamma_{crit} \geq 16.88^\circ$ and the second a $\gamma_{crit} = 15.71^\circ$. Figure 9 shows that $u(A)$ and $|du(A)/d\gamma|$ become large as γ approaches 15° , which is consistent with these predictions. It also shows that the γ_{crit} due to the ellipse's curvature cannot be much larger than 16.88° . This illustrates that the lower bound given by Theorem 3 is again close to γ_{crit} .

Finally, for the case $b=0.60$ with $\kappa=0$, the coarseness of the mesh caused the solution of the discrete system of equations to differ somewhat from those for the cases $b=0.20$ and 0.33 . The sharp corner should give a γ_{crit} of 8.79° for the 11×6 mesh and 4.55° for the 21×11 mesh. The lower bound on γ_{crit} due to the ellipse's curvature is 0.12° . However, Fig. 9 shows that although $u(A)$ increases as γ approaches 0° , $|du(A)/d\gamma|$ decreases. When the mesh was refined from 11×6 to 21×11 , $u(A)$ increased by 9%, 7%, 4%, and 2%, at $\gamma = 0^\circ, 5^\circ, 10^\circ$, and 15° , respectively. The relatively larger increase for 0° and 5° than for 15° shows the effects of the corner, but not as dramatically as for the $b=0.20$ case. The coarseness of the mesh is shown by the change in $u(B)$ when the

mesh was refined. It changed by 6%, 5%, 4%, and 3%, at $\gamma = 0^\circ, 5^\circ, 10^\circ$, and 15° , respectively. In contrast, for the case $b = 0.20$ with $\kappa = 0$, $u(B)$ changed by only 0.6% when the mesh was refined.

9. CALCULATING CAPILLARY SURFACES ON CROSS SECTIONS WITH CORNERS

A cylinder whose cross section has a corner, as in Fig. 11A, will have a critical contact angle. If the interior angle at the corner is 2α , then $\gamma_{\text{crit}} = 90^\circ - \alpha$. There are no solutions to Eqs. (1) and (2) for $\kappa = 0$ and $\gamma < \gamma_{\text{crit}}$. Solutions exist for $\kappa \neq 0$ and $\gamma < \gamma_{\text{crit}}$, but the height goes to infinity at the corner. It would be difficult to compute such a surface numerically over the entire cross section. Instead, the cross section is divided into two regions, as with curve AA' of Fig. 11A. One is a small region Ω_c that includes the corner; the other Ω_r is the remainder of the cross section. The asymptotic form of the surface near the corner region is known. The surface on the remainder Ω_r can be calculated numerically, with the boundary condition that it match the asymptotic solution along the curve AA' .

The boundary data are the values of the function $(\hat{n} \cdot \nabla u)/W$ at each point on the boundary. W is the function $(1 + |\nabla u|^2)^{1/2}$, and $\hat{n}$ is the outward directed normal at the boundary. $(\hat{n} \cdot \nabla u)/W$ is $\cos \gamma$ at the cylinder wall. It is zero on boundaries that are lines of reflection symmetry. It is matched with that of the asymptotic solution along the boundary curve AA' .

The surface in a neighborhood of the corner has the asymptotic form [3]

$$u(\rho, \theta) \sim u_0(\rho, \theta) + v(\rho, \theta) \quad . \quad (10)$$

where u_0 is a function of $O(1)$ and

$$v(\rho, \theta) = \frac{1}{\kappa \rho} [q \cos \gamma - (1 - q^2 \sin^2 \theta)^{1/2}] . \quad (11)$$

The quantities ρ and θ are polar coordinates of a point on the cross section; ρ is the radial distance from the corner, and θ is the angle measured from the bisector of the corner angle. These are shown in Fig.

11B. The quantity q is

$$q = \frac{\cos \gamma}{\sin \alpha} = \frac{\cos \gamma}{\cos \gamma_{\text{crit}}} \quad (12)$$

For $\rho \ll 1$, we have $u_0 \ll v$.

The boundary condition function $(\hat{n} \cdot \nabla u)/W$ can be broken into two factors, a magnitude and the inner product of two unit vectors.

$$\frac{\hat{n} \cdot \nabla u}{W} = \frac{|\nabla u|}{W} \frac{\hat{n} \cdot \nabla u}{|\nabla u|} . \quad (13)$$

We do not know the order of ∇u_0 , but we know that $|\nabla v|$ is $O(1/\rho^2)$, so that in general $|\nabla u|$ also must be at least $O(1/\rho^2)$. Consequently,

$$\begin{aligned} \frac{|\nabla u|}{W} &= 1 - \frac{1}{2|\nabla u|^2} + \dots \\ &= 1 - O(\rho^4) . \end{aligned} \quad (14)$$

Thus if the curve AA' is sufficiently near the corner, then $|\nabla u|/W$ is approximately 1.

We next consider the factor $(\hat{n} \cdot \nabla u)/|\nabla u|$. The quantity $\nabla u/|\nabla u|$ is a unit vector normal to a level curve of u . If we choose the curve AA' to be this level curve, then $\hat{n} = \nabla u/|\nabla u|$, and so $(\hat{n} \cdot \nabla u)/|\nabla u|$ will be 1. The level curve of u is not known, but for small ρ we have $u_0 \ll v$, so a level curve of u is approximately a level curve of v . We shall

choose the curve AA' to be a level curve of v ; thus the factor $(\hat{n} \cdot \nabla u)/|\nabla u|$ will be approximately 1.

The level curves of v are a family of circles, which depend on the contact angle γ . The radius of a circle is $1/\kappa v$, and its center lies on the bisector of the corner at a distance $q/\kappa v$ from the corner. The circle intersects the cross section of the cylinder wall at an angle γ , as shown in Fig. 11C.

Let u denote the solution of Eqs. (1) and (2) on the entire cross section with $(\hat{n} \cdot \nabla u)/W = \cos \gamma$ at the cylinder wall. Let u_r denote the solution of (1) and (2) on Ω_r with $(\hat{n} \cdot \nabla u)/W = \cos \gamma$ at the cylinder wall and with $(\hat{n} \cdot \nabla u)/W = 1$ on the curve AA' . It is shown in Ref. 8 that u_r is an upper bound to u at each point in Ω_r .

10. SQUARE CROSS SECTION WITH $\kappa=1$

The capillary surface over a square cross section was calculated for $\gamma=30^\circ$ and $\kappa=1$ by deleting the corner as described in the previous section. The value of γ_{crit} for a square is 45° . The calculation was performed on 1/4 of a 2×2 square. The 9×9 mesh that was used is shown in Fig. 12. The boundary condition function $(\hat{n} \cdot \nabla u)/W$ is 0 along the reflection symmetry boundary BOB' . It is $\cos 30^\circ$ along the edges BA and $B'A'$, and is approximately 1 on the curve AA' that divides the corner from the remainder of the cross section. Curve AA' is composed of eight straight line segments, which approximate a level curve of v for $\gamma=30^\circ$.

The heights of the capillary surface along the edge AB and along

the diagonal CO are shown in Fig. 13. The height is taken to be zero at the center of the square, O. The height is approximately 1.80 on the boundary curve AA' and is almost constant along the curve. It differs by only 0.0062 between the endpoint A and the midpoint C of the curve.

The point B is the midpoint of the edge of the full square. The height of the capillary surface $u(B)$ is shown in Fig. 14 for $\kappa=1$ and $\gamma=30^\circ, 45^\circ, 50^\circ, 55^\circ$, and 60° . The four surfaces with $\gamma \geq \gamma_{crit}$ were calculated on a 6×6 mesh with uniform spacing. In the case $\kappa=0$, discussed previously, it was found that this mesh gives an accurate value for $u(B)$, although the height at the corner is inaccurate for $\gamma=45^\circ$. It is interesting to note that $u(B)$ changes almost uniformly over the range $30^\circ \leq \gamma \leq 90^\circ$. It does not change rapidly near $\gamma=45^\circ$ or in the range $30^\circ \leq \gamma \leq 45^\circ$. Although the fluid is drawn up to an infinite height in the corner, our calculation indicates that this does not affect dramatically the height at the midpoint.

11. CIRCULAR CROSS SECTION WITH A REENTRANT NOTCH

Capillary surfaces were calculated for a circular cross section with four rectangular reentrant notches as shown in Fig. 15A. The calculation was performed on $1/8$ of the cross section, which is shown in Fig. 15B. The circle has radius 1. The notch extends inward to a depth 0.2 on the axis and has half-width 0.2. The corner, point G of Fig. 15B, corresponds to a γ_{crit} of 50.77° .

A series of exploratory calculations were made with 9×8 meshes for $\kappa=1.0$ and $\gamma=0^\circ, 15^\circ, 30^\circ, 45^\circ$, and 60° . Figures 16 and 17 show the 9×8 meshes used for $\gamma=60^\circ$ and $\gamma=0^\circ$. The case $\kappa=1.0$ and $\gamma=0^\circ$

was calculated also with the 13×12 mesh shown in Fig. 18. The cases with $\gamma < \gamma_{\text{crit}}$ were calculated by deleting the corner as described previously.

The asymptotic solution of Eqs. (1) and (2) is not known for a corner which consists of a straight line intersecting a circular arc, as in Fig. 15C. However, the arc GHE differs only slightly from its chord GJE. The asymptotic solution for the corner which has CGJE for its cylinder wall is the function $v(\rho, \theta)$ defined previously. For our calculations, the dividing curve CDE was chosen to be a level curve of this $v(\rho, \theta)$.

Figures 19 and 20 show level curves of the numerical solutions for the 60° and 0° cases. In the 60° case, the fluid slopes gently up toward the cylinder wall and the corner G. In the 0° case, the fluid is drawn strongly up into corner G.

Figure 21 shows the variation of the height of the capillary surface with the contact angle γ , at various points on the cross section. The height is taken to be zero at the center of the circle, point O. The 13×12 and 9×8 meshes give somewhat different values for the surface height for $\gamma = 0^\circ$. The heights at points A, B, and F differ by the fractions $0.05/0.76$, $0.02/1.52$, and $0.07/1.42$. The meshes do not give high accuracy because only a few points are used to approximate the corner region, where the gradient is steep. However, these calculations show the general nature of the solution. Greater accuracy can be obtained by refining the mesh and moving the level curve CDE nearer the corner G.

Figure 22 shows the height of the surface for $\gamma = 60^\circ$ as a function of the arc length along the cylinder wall ABCGEF. It shows also the heights of the surfaces for $\gamma = 0^\circ$ and 30° along the wall from point A

to C and from E to F. The apparent discontinuity in the slope of the $\gamma = 0^\circ$ surface at point B results not from an actual discontinuity, but because the cylinder wall changes direction by 90° at B. The slopes on one side and the other of the point B in Fig. 22 refer to two different directions. For the 60° case, the fluid rises only slightly from 0.305 at F to 0.506 at corner G. In the 0° and 30° cases, it rises steeply as G is approached.

CDE is a level curve of v . It is a circular arc that intersects the cylinder wall at an angle γ . The curve CDE was approximated by 4 straight line segments of the 9×8 mesh and by 8 segments of the 13×12 mesh. Table 6 shows the calculated height along these level curves.

TABLE 6. Calculated height along CDE.

γ	Mesh	$u(C)$	$u(D)$	$u(E)$
0°	13×12	8.24	9.83	8.25
15°	9×8	5.36	5.76	5.16
30°	9×8	2.59	2.65	2.48
45°	9×8	0.930	0.933	0.913

The height is quite level along CDE for the 45° case. However, it increases by 16% at the middle of the curve for the 0° case. For this case, the level curve of u is less bowed toward the corner than the level curve of v . The level curves of u asymptotically approach circular arcs as their distance to the corner approaches zero, because u_0/v approaches 0. However, the point C is not very close to the corner. It is almost halfway from the corner G to point B. If a finer mesh is used, CDE can be chosen nearer the corner, where the level curve of v more closely approximates that of u .

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Fig. 1. Cross section of a cylinder.

(XBL 775-947)

Fig. 2. Height u of the capillary surface as a function of the distance y along the edge $x=1.0$ for $\kappa=0$ and $\gamma=45^\circ, 50^\circ, 55^\circ, \text{ and } 60^\circ$.

(XBL 776-1116)

Fig. 3. Height u of the capillary surface as a function of the contact angle γ on the edge $x=1.0$ for $\kappa=0$ and $y=0.0, 0.6, 0.8$, and 1.0 . (XBL 775-954)

Fig. 4. One-fourth ellipse with $a=1.0$ and $b=0.6$ showing values of (x,y) at the corners and values of L or M on the edges. (XBL 775-948)

Fig. 5. 11×6 mesh for a 1/4 ellipse with $a = 1.0$ and $b = 0.33$. (XBL 776-1217)

Fig. 6. 11×6 mesh for a 1/4 ellipse with $a = 1.0$ and $b = 0.20$. (XBL 776-1219)

Fig. 7. 21×11 mesh for a 1/4 ellipse with $a = 1.0$ and $b = 0.20$. (XBL 776-1218)

Fig. 8. Level curves of the capillary surface for $\gamma=60^\circ$, $a=1.0$, and $b=0.33$. (XBL 776-1126)

Fig. 9. Height u of the capillary surface at the point A as a function of the contact angle γ for $\kappa=0$ and $b=0.60$, 0.33 , and 0.20 and for $\kappa=1$ and $b=0.20$. (XBL 775-953)

Fig. 10. Height u of the capillary surface at the point B as a function of the contact angle γ for $\kappa = 0$ and $b = 0.60$, 0.33 , and 0.20 and for $\kappa = 1$ and $b = 0.20$. (XBL 776-1118)

Fig. 11. Cross section of a cylinder and details.

(XBL 775-950)

Fig. 12. 9x9 mesh for a 1/4 square with the corner deleted.
(XBL 776-1220)

Fig. 13. Height u of the capillary surface along the edge and the diagonal, respectively, as a function of the distance ρ from the corner. (XBL 776-1120)

Fig. 14. Height u of the capillary surface at the midpoint B of the edge of the full square as a function of contact angle γ . (XBL 776-1115)

Fig. 15. Cross section of a cylinder with a reentrant notch, and details.
(XBL 775-951)

Fig. 16. 9×8 mesh for a cylinder with a reentrant notch for $\gamma = 60^\circ$.
(XBL 776-1123)

Fig. 17. 9×8 mesh for a cylinder with a reentrant notch for $\gamma = 0^\circ$.
(XBL 776-1122)

Fig. 18. 13×12 mesh for a cylinder with a reentrant notch for $\gamma = 0^\circ$.
(XBL 776-1125)

Fig. 19. Level curves of the capillary surface for $\gamma = 60^\circ$.
(XBL 776-1124)

Fig. 20. Level curves of the capillary surface for $\gamma=0^\circ$.
(XBL 776-1121)

Fig. 21. Height u of the capillary surface at points A, B, E, and F as a function of contact angle γ . (XBL 775-952)

Fig. 22. Height u of the capillary surface as a function of arc length along the cylinder wall for $\gamma = 0^\circ$, 30° , and 60° .
(XBL 776-1119)

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